Influence of Prior Covariance Structure on Inverse Estimates of CO2 Fluxes in Los Angeles Basin

Vineet Yadav
Jet Propulsion Laboratory, California Institute of Technology

JSM 2019 (Denver)
7/31/2019

Jet Propulsion Laboratory
California Institute of Technology

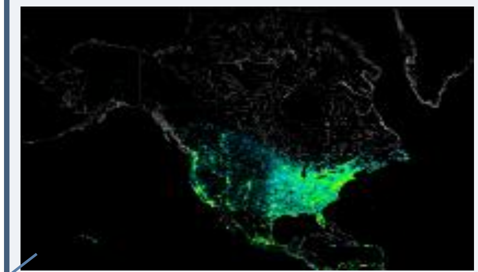
Layout of the presentation

- Formulation of atmospheric Inverse Models
- Criteria for assessing inverse models
- Choices that impact inverse models
- Types of prior covariance used in inverse models
- The phenomenon for which prior covariance needs to be defined
- Role of prior covariance in inverse output
- Case Studies:
  - Regional: North America
  - Urban: Los Angeles

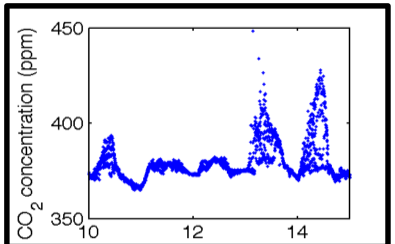
Statistical Approach to Atmospheric Inversions

Atmospheric Inversions: Components of (linear) Statistical Model

FF Fluxes



CO_2 Observations



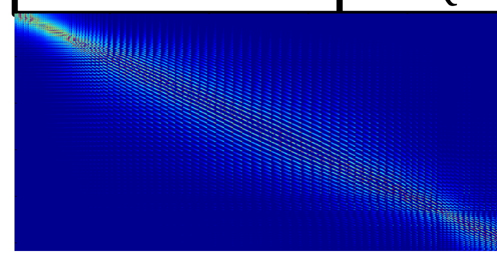
Measurement Error Covariance | $\boldsymbol{\varepsilon}_R$

$$L_{\mathbf{s},\boldsymbol{\beta}} = \frac{1}{2}(\mathbf{z} - \mathbf{Hs})^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{z} - \mathbf{Hs}) + \frac{1}{2}(\mathbf{s} - \mathbf{s}_p)^{\mathrm{T}}\mathbf{Q}^{-1}(\mathbf{s} - \mathbf{s}_p) \qquad (1)$$

Transport Model

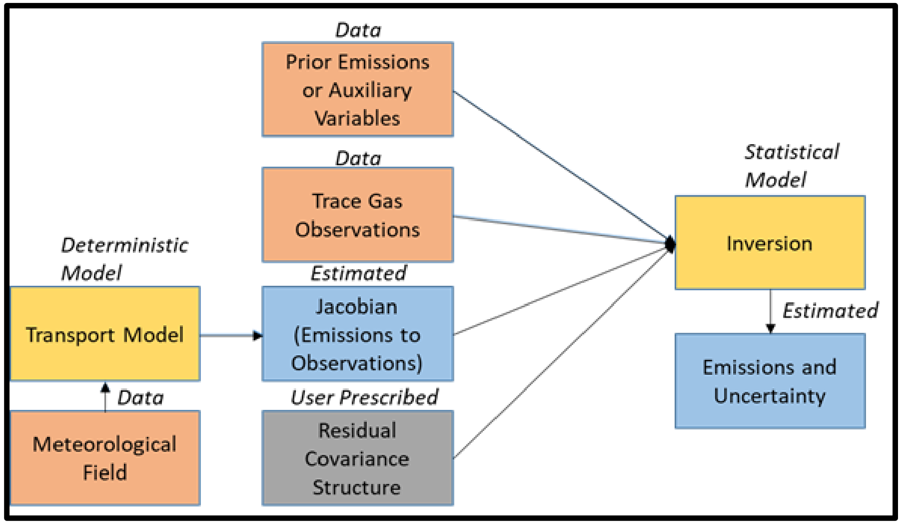
CO2 Emissions

Prior Covariance | $\boldsymbol{\varepsilon}_Q$



Flavors of Atmospheric (linear) Inverse Models

Inverse Process



Bayesian

$$L_{\mathbf{s}} = \frac{1}{2}(\mathbf{z}-\mathbf{Hs})^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{z}-\mathbf{Hs}) + \frac{1}{2}(\mathbf{s}-\mathbf{s}_p)^{\mathrm{T}}\mathbf{Q}^{-1}(\mathbf{s}-\mathbf{s}_p) \quad (2)$$

Geostatistical

$$L_{\mathbf{s},\boldsymbol{\beta}} = \frac{1}{2}(\mathbf{z}-\mathbf{Hs})^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{z}-\mathbf{Hs}) + \frac{1}{2}(\mathbf{s}-\mathbf{X}\boldsymbol{\beta})^{\mathrm{T}}\mathbf{Q}^{-1}(\mathbf{s}-\mathbf{X}\boldsymbol{\beta}) \quad (3)$$

Another Formulation

$$L_{\mathbf{s},\boldsymbol{\beta},\mathbf{u}} = (\mathbf{z}-\mathbf{Hs})^{T}\mathbf{R}^{-1}(\mathbf{z}-\mathbf{Hs}) + (\mathbf{s}-\mathbf{X}\boldsymbol{\beta}-\mathbf{Mu})^{T}\mathbf{Q}^{-1}(\mathbf{s}-\mathbf{X}\boldsymbol{\beta}-\mathbf{Mu}) + \mathbf{u}^{T}\mathbf{P}^{-1}\mathbf{u} \quad (4)$$

Criteria for assessing an inverse model (other than Uncertainty Reduction)

Correlation Coefficient and RMSE

$$corr(\mathbf{z}, \mathbf{H}\hat{\mathbf{s}}) \tag{5}$$

$$RMSE = \sqrt{\frac{\mathbf{1}^{\mathrm{T}}(\mathbf{z} - \mathbf{H}\hat{\mathbf{s}})^{\circ 2}}{n}} \tag{6}$$

Hat Matrix and Cross Validation

$$\mathbf{h} = \mathbf{H}\mathbf{s}_p\left((\mathbf{H}\mathbf{s}_p)^T\left(\mathbf{H}\mathbf{Q}\mathbf{H}^{\mathrm{T}} + \mathbf{R}\right)^{-1}\mathbf{H}\mathbf{s}_p\right)^{-\mathbf{1}}(\mathbf{H}\mathbf{s}_p)^T\left(\mathbf{H}\mathbf{Q}\mathbf{H}^{\mathrm{T}} + \mathbf{R}\right)^{-1} \tag{7}$$

$$cv = \frac{1}{n}\sum_{i=1}^{N}\left(\frac{e_i}{1 - h_{ii}}\right)^2 \tag{8}$$

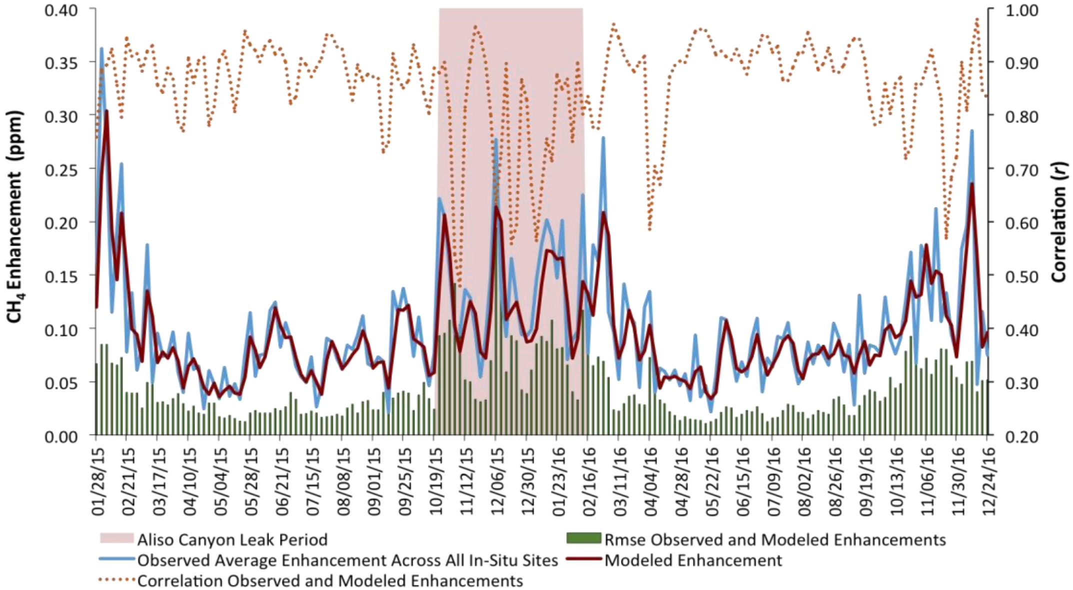
Averaging Kernel Matrix

$$\mathbf{G} = \mathbf{Q}\mathbf{H}^T\left(\mathbf{H}\mathbf{Q}\mathbf{H}^{\mathrm{T}} + \mathbf{R}\right)^{-1}\mathbf{H} \tag{9}$$

Reduced Chi-Square Statistic

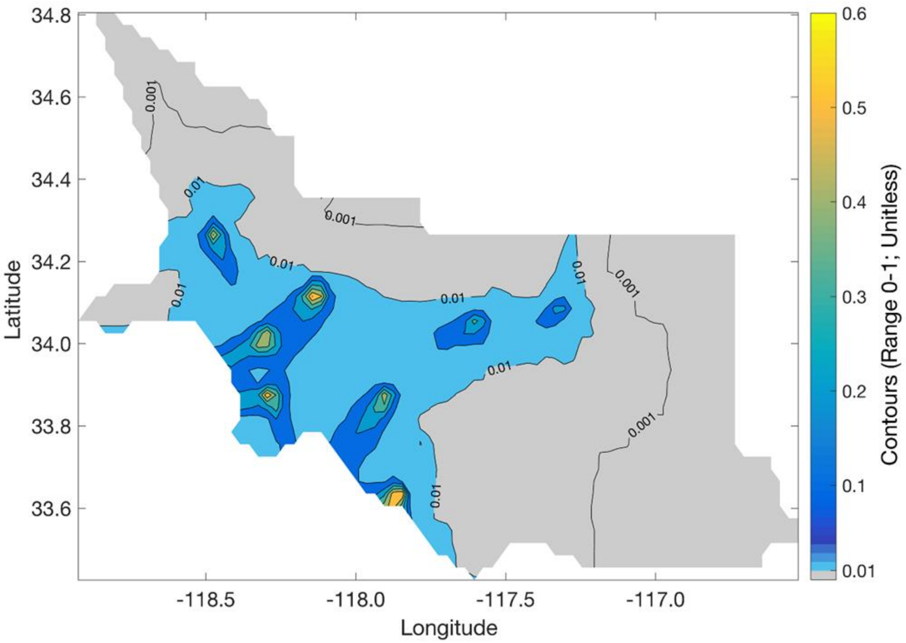
$$\chi^2_{red} = \frac{(\mathbf{z} - \mathbf{H}\hat{\mathbf{s}})^T\mathbf{R}^{-1}(\mathbf{z} - \mathbf{H}\hat{\mathbf{s}}) + (\mathbf{s} - \mathbf{s}_p)^T\mathbf{Q}^{-1}(\mathbf{s} - \mathbf{s}_p)}{n} \tag{10}$$

Criteria for assessing an inverse model: Examples



Correlation and RMSE

Averaging Kernel



Sensitivity Analysis

- How to determine which factor played most important role in influencing estimates of fluxes ?
- There are multiple ways to do this but partial derivatives provide a complete framework to do this.

$$\boxed{\boldsymbol{\Psi} = \left(\mathbf{HQH}^{\mathrm{T}} + \mathbf{R}\right)}$$

$$\frac{\partial \hat{\mathbf{s}}}{\partial \mathbf{z}} = \underbrace{\mathbf{QH}^{T}\boldsymbol{\Psi}^{-1}}_{Kalman\ Gain} \tag{11}$$

$$\frac{\partial \hat{\mathbf{s}}}{\partial \mathbf{Q}} = \mathbf{H}^{T}\boldsymbol{\Psi}^{-1}\left(\mathbf{z} - \mathbf{HS}_{prior}\right) \otimes \mathbf{I}_{k} - \mathbf{H}^{T}\boldsymbol{\Psi}^{-1}\left(\mathbf{z} - \mathbf{HS}_{prior}\right) \otimes \mathbf{H}^{T}\boldsymbol{\Psi}^{-1}\mathbf{HQ} \tag{12}$$

$$\frac{\partial \hat{\mathbf{s}}}{\partial \mathbf{R}} = \boldsymbol{\Psi}^{-1}\left(\mathbf{z} - \mathbf{HS}_{prior}\right) \otimes \boldsymbol{\Psi}^{-1}\mathbf{HQ} \tag{13}$$

$$\overbrace{\Delta\,\hat{\mathbf{s}}}^{\substack{Normalized\\ Sensitivity}} = \frac{\kappa_i^{o}}{\hat{\mathbf{s}}(\kappa^{o})} \times \left[\frac{\partial \hat{\mathbf{s}}}{\partial \kappa_i^{o}}\right] \tag{14}$$

Importance of Prior Covariance Matrix

Impact of Prior Covariance (North America Example)

Separable Exponential Space-Time

$$\mathbf{Q} = \sigma^2 \left[\exp\left(\frac{-\boldsymbol{d}_{temporal}}{l_{temporal}} \right) \otimes \exp\left(\frac{-\boldsymbol{d}_{spatial}}{l_{spatial}} \right) \right] \quad (10)$$

Spatially dependent error variance

$$\mathbf{Q} = \left(a \begin{bmatrix} k_1 & 0 & 0 \\ 0 & . & 0 \\ 0 & 0 & k_r \end{bmatrix} + b \begin{bmatrix} 1 & 0 & 0 \\ 0 & . & 0 \\ 0 & 0 & 1 \end{bmatrix} \right) \quad (11)$$

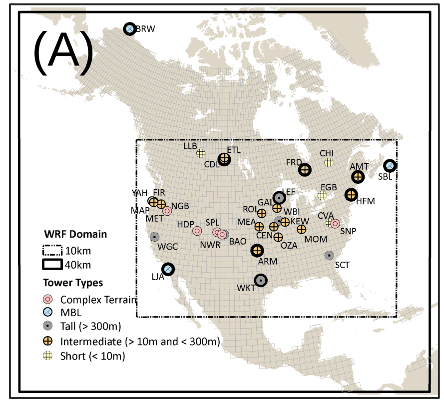
Assessment: BIC

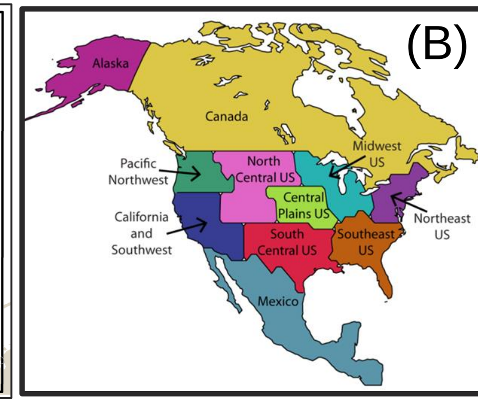
$$BIC = \underbrace{RSS + \ln\left|(\mathbf{HQH}^T + \mathbf{R})^{-1}\right|}_{log\ likelihood} + \underbrace{p \ln(n)}_{penalty\ term} \quad (12)$$

Impact of Prior Covariance (North America Example II)

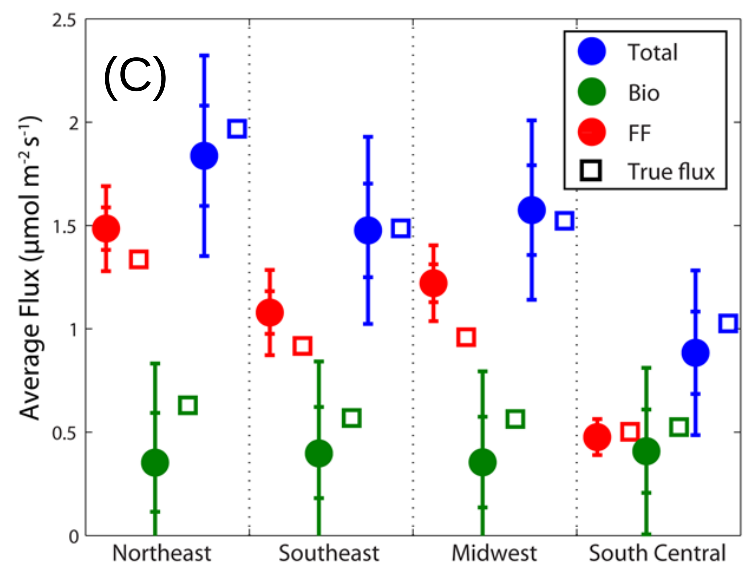
Details of the Case Study:

- Inversion Area: North America
- Inversion Time Period: 2008
- Resolution: 3-Hourly, $1^{o} \times 1^{o}$
- Observations: 35 in-situ towers
- Simulation Study: True Fluxes were known
- Prior Covariance Assessed:
    1. Night Lights
    2. Population Density
    3. Urban Area
    4. FF Inventory
    5. Separable Exponential Covariance





A. Study Area and In-Situ Towers
B. Flux Aggregation Area
C. Results from the case study



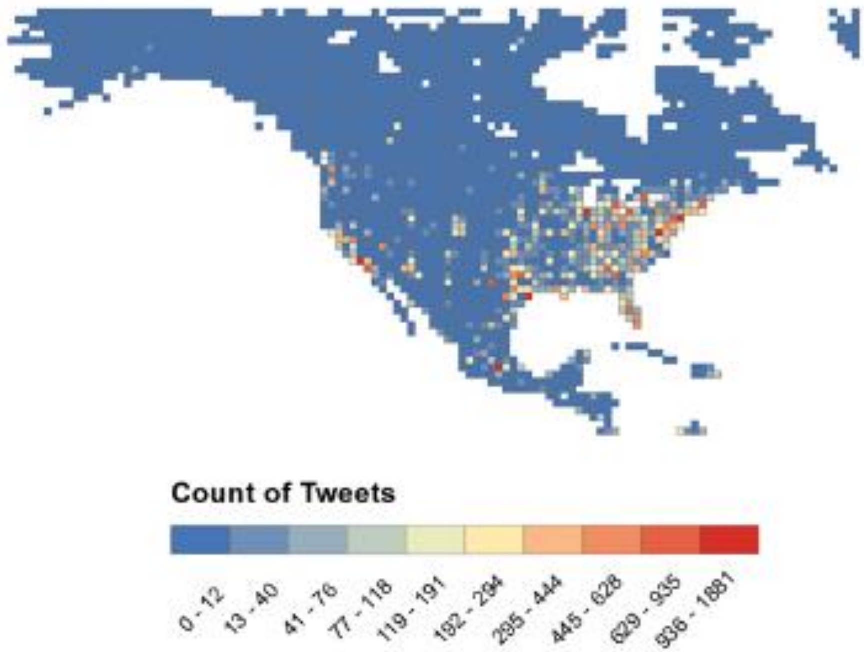
Results:

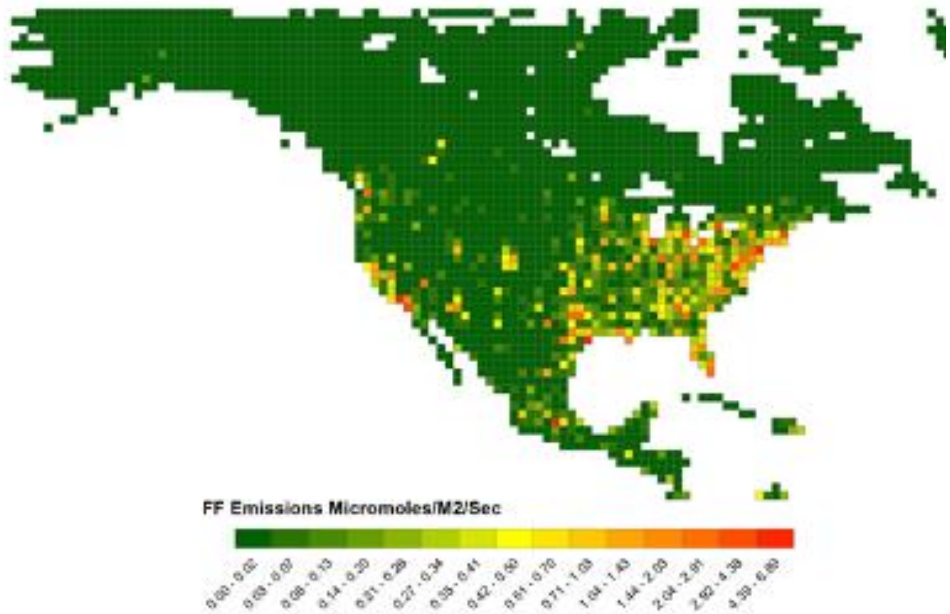
- FF Inventory based covariance considerably better than other covariance structures

Yadav et. al. (JGR-Atmospheres 2016)

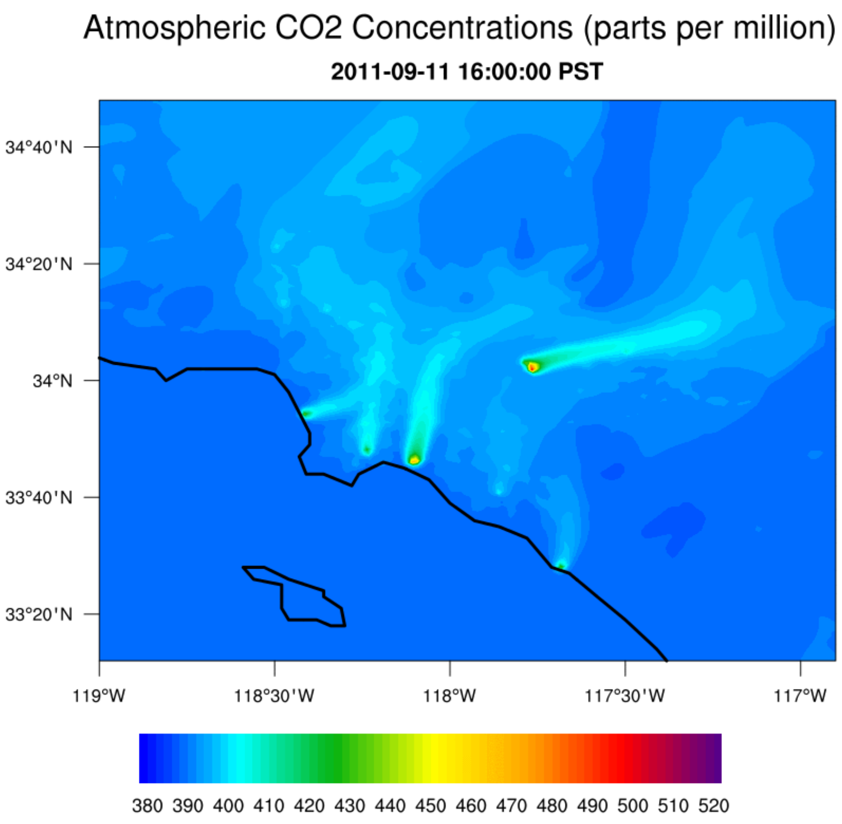
Impact of Prior Covariance (North America Example III)

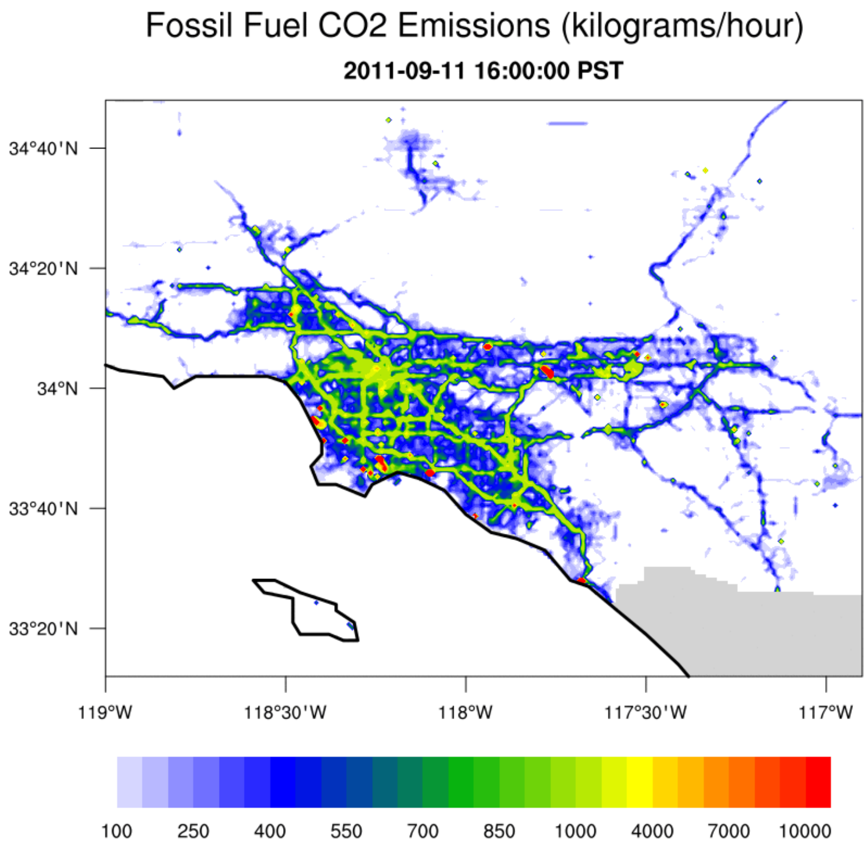
Work in Progress: Estimating Fossil Fuel Emissions By Using Twitter Feeds





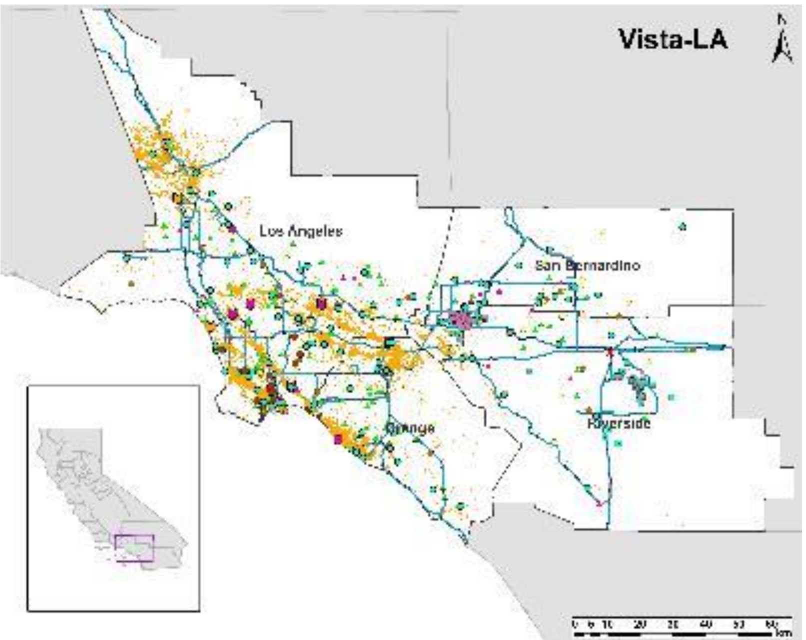
Observations to Fluxes: Why is prior covariance so important in urban areas (Example from Los Angeles)



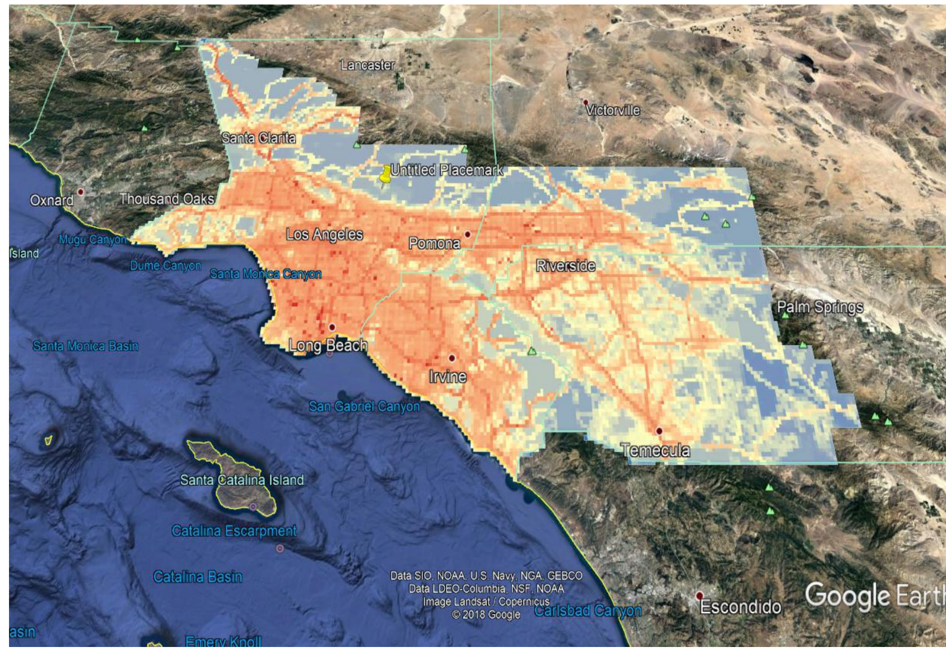


Observations to Fluxes: Why is prior covariance so important in urban areas (Example from Los Angeles) II

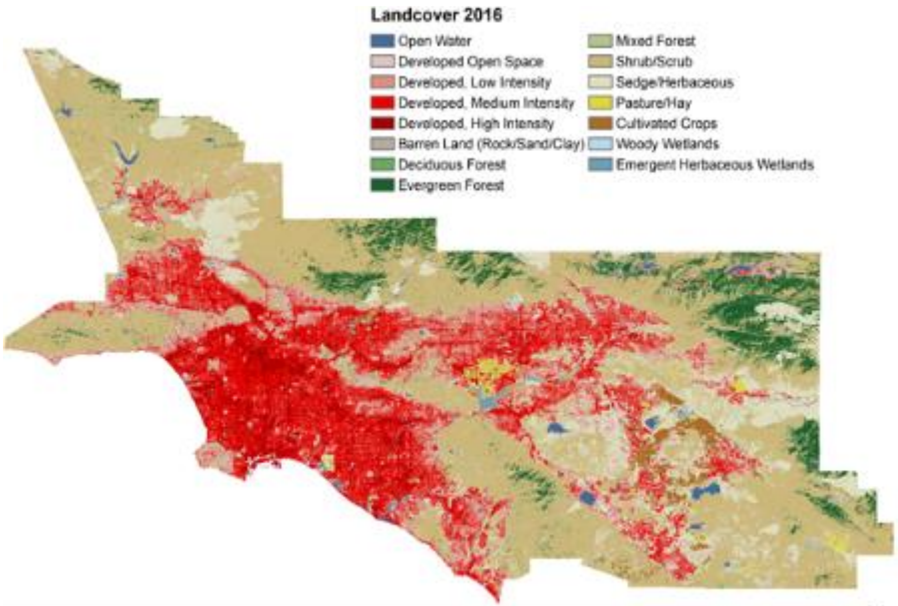
Distribution of Methane Emitting Infrastructure

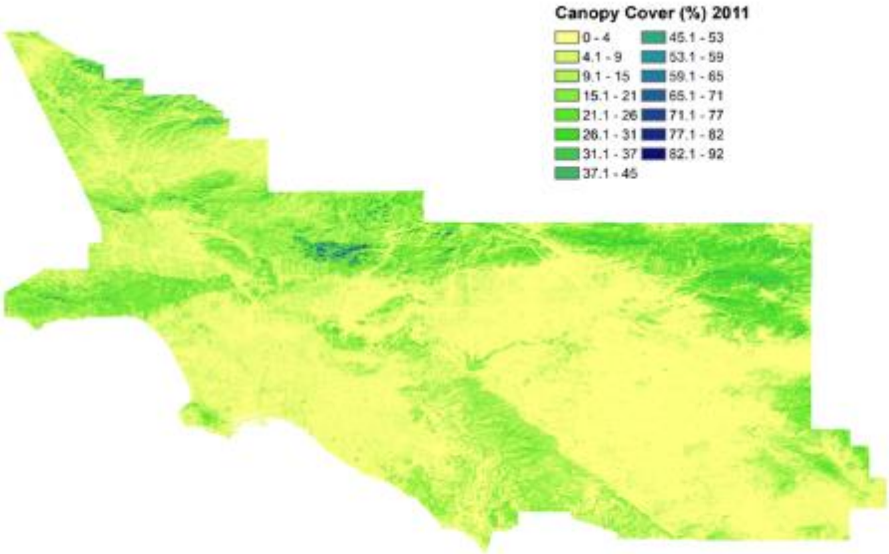


Hourly Carbon dioxide emissions from Los Angeles



Observations to Fluxes: Why is prior covariance so important in urban areas (Example from Los Angeles) III





Behavior of different covariance formulations

Details of the Case Study:

- Inversion Area: Los Angeles
- Inversion Time Period: 2015
- Resolution: 4-day, 3km
- Observations: 6 in-situ towers
- Real data Study:
- Prior Covariance Assessed:
    1. FF Inventory (diagonal)
    2. Separable Exponential Covariance
    3. Temporal correlation and diagonal spatial

Results

- Correlation length in Space is non present
- Correlation length is considerably larger in time

Conclusions and Future Steps

- Implement proposed covariance structures for estimating fluxes

$$\mathbf{Q} = \sigma^2 \left[\exp\left(\frac{-\boldsymbol{d}_{temporal}}{l_{temporal}} \right) \otimes \left(a \begin{bmatrix} k_1 & 0 & 0 \\ 0 & . & 0 \\ 0 & 0 & k_r \end{bmatrix} + b \begin{bmatrix} 1 & 0 & 0 \\ 0 & . & 0 \\ 0 & 0 & 1 \end{bmatrix} \right) \right] \tag{13}$$

- Include observations from multiple instruments

- Perform sensitivity analysis
- Use real time social media to better define temporal covariance model